Higher Order Hybrid Monte Carlo at Finite Temperature

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Abstract

The standard hybrid Monte Carlo algorithm uses the second order integrator at the molecular dynamics step. This choice of the integrator is not always the best. We study the performance of the hybrid Monte Carlo algorithm for lattice QCD with higher order integrators in both zero and finite temperature phases and find that in the finite temperature phase the performance of the algorithm can be raised by use of the 4th order integrator.

1 Introduction

In lattice QCD the hybrid Monte Carlo (HMC) algorithm [1] is widely used for simulations of even flavor of quarks[1]. These simulations are usually difficult tasks, especially at small quark masses where the computational cost of the matrix solver which is the most time consuming part of the HMC algorithm grows. In order to obtain reliable results within limited computer resources it is important to find an efficient way to implement the HMC algorithm so that the total computational cost of the algorithm is minimized [3].

The basic idea of the HMC is a combination of 1) molecular dynamics and 2) Metropolis test. Usually the second order leapfrog integrator is used at the molecular dynamics (MD) step. The integrator causes $\mathcal{O}(\Delta t^3)$ integration errors, where Δt denotes the step-size. Due to the integration errors the Hamiltonian is not conserved. The errors introduced by this integrator have to be removed by the Metropolis test, i.e. accept the new configuration with a probability $\sim \min(1, \exp(-\Delta H))$ where $\Delta H = H_{new} - H_{old}$ is an energy difference between the starting Hamiltonian H_{old} and the new Hamiltonian H_{new} at the end of the trajectory.

The acceptance at the Metropolis step depends on the magnitude of the energy difference induced by the integration errors. If a higher order integrator is used at the MD step, the integration errors can be reduced. Therefore one may easily imagine that the performance of the HMC increases with the higher order integrator. However this is not always true since the higher order integrator has more arithmetic operations than the lower one and this might decrease the performance. The total performance should be measured by taking account of two effects: acceptance and the number of arithmetic operations. In Ref.[4] the performance of the higher order integrator at zero temperature ($\beta = 0$) was studied systematically and it turned out that for the simulation parameters used for the current large-scale simulations the 2nd order integrator is the best one. The main reason why the higher order integrators are not so effective is that the energy difference caused by the errors of the higher order integrator increases more rapidly than that of the lower one as the quark mass decreases. In Ref.[5] it is shown that at finite temperature the quark mass dependence of the energy difference is small. If so, the conclusion of Ref.[4] might change at finite temperature. In this letter we test higher order integrators at finite temperature and demonstrate that they can actually perform better than the lower order.

2 Higher order integrator

In this section we define higher order integrators studied here. Our definition is parallel to that of Ref.[4]. Let H be a Hamiltonian given by

$$H = \frac{1}{2}p^2 + S(q) \tag{1}$$

[1]Odd-flavor simulations of the HMC algorithm are also possible by modifying the Hamiltonian [2].

where $q = (q_1, q_2, ...)$ and $p = (p_1, p_2, ...)$ are coordinate variables and conjugate momenta respectively. $S(q)$ is a potential term of the system considered. For the lattice QCD, q correspond to link variables and $S(q)$ consists of gauge and fermion actions.

In the MD step we solve Hamilton's equations of motion,

$$\begin{cases} \dfrac{dq_i}{dt} &= \dfrac{\partial H}{\partial p_i} \\ \dfrac{dp_i}{dt} &= -\dfrac{\partial H}{\partial q_i}. \end{cases} \tag{2}$$

In general these equations are not solvable analytically. Introducing a step-size Δt, the discretized version of the equations are solved. In the conventional HMC simulations the 2nd order leapfrog scheme, which causes $\mathcal{O}(\Delta t^3)$ step-size error, is used to solve the equations. This scheme is written as

$$\begin{cases} q(t + \frac{\Delta t}{2}) &= q(t) + \frac{\Delta t}{2} p(t) \\ p(t + \Delta t) &= p(t) - \Delta t \dfrac{\partial S(q(t + \frac{\Delta t}{2}))}{\partial q} \\ q(t + \Delta t) &= q(t + \frac{\Delta t}{2}) + \frac{\Delta t}{2} p(t + \Delta t). \end{cases} \tag{3}$$

Eq.(3) forms an elementary MD step. This elementary MD step is performed repeatedly N times. The trajectory length τ is given by $\tau = N \times \Delta t$.

Any integrator which satisfies two conditions: 1)time reversible and 2)area preserving can be used for the MD step of the HMC. These conditions are needed to satisfy the detailed balance. When we use the Lie algebraic formalism [6, 7, 8, 9] we can easily construct higher order integrators which satisfy the above conditions. From the Lie algebraic formalism we find that higher order integrators can be constructed by combining lower order integrators. Let $G_{2nd}(\Delta t)$ be an elementary MD step of the 2nd order integrator with a step-size Δt. The 4th order integrator $G_{4th}(\Delta t)$ is constructed from a product of *three* 2nd order integrators as [6, 7, 8, 9, 10]

$$G_{4th}(\Delta t) = G_{2nd}(a_1 \Delta t) G_{2nd}(a_2 \Delta t) G_{2nd}(a_1 \Delta t), \tag{4}$$

where the coefficients a_i are given by

$$a_1 = \frac{1}{2 - 2^{1/3}}, \tag{5}$$

$$a_2 = -\frac{2^{1/3}}{2 - 2^{1/3}}. \tag{6}$$

Eq.(4) means that there are three elementary MD steps: (i) first we integrate the equations by eq.(3) with a step-size of $a_1 \Delta t$, (ii) then proceed the 2nd order integration with a step-size of $a_2 \Delta t$, (iii) finally integrate the equations with a set-size of $a_1 \Delta t$. After performing these three elementary MD steps sequentially we obtain the

4th order integrator with the step-size Δt. This construction scheme can be generalized to the higher *even*-order integrators. The $(2k+2)$-th order integrator is given recursively by

$$G_{2k+2}(\Delta t) = G_{2k}(b_1\Delta t)G_{2k}(b_2\Delta t)G_{2k}(b_1\Delta t), \tag{7}$$

where the coefficient b_i are

$$b_1 = \frac{1}{2 - 2^{1/(2k+1)}} \tag{8}$$

$$b_2 = -\frac{2^{1/(2k+1)}}{2 - 2^{1/(2k+1)}}. \tag{9}$$

Compared with the 2nd order integrator, the computational cost of the n-th order one constructed from eq.(7) grows as $3^{n/2-1}$. For instance the 6th order integrator has 9 times more arithmetic operations than those of the 2nd order one. Yoshida [8] found *three* parameter sets of 6th order integrators with less arithmetic operations (Table.1). Yoshida's 6th order integrators consist of *seven* G_{2nd}'s as

$$\begin{aligned} G_{6th}(\Delta t) &= G_{2nd}(w_3\Delta t)G_{2nd}(w_2\Delta t)G_{2nd}(w_1\Delta t)G_{2nd}(w_0\Delta t) \\ &\quad \times G_{2nd}(w_1\Delta t)G_{2nd}(w_2\Delta t)G_{2nd}(w_3\Delta t). \end{aligned} \tag{10}$$

In Ref.[4] these 6th order integrators were examined and one of three parameter sets, denoted by $Y1$, was found to give smaller integration errors than those of others. In this study the parameter set $Y1$ (see Table.1) is used for the 6th order integrator.

	Y1	Y2	Y3
w_1	-0.117767998417887e-1	-0.213228522200144e+1	0.152886228424922e-2
w_2	0.235573213359357e+0	0.426068187079180e-2	-0.214403531630539e+1
w_3	0.784513610477560e+0	0.143984816797678e+1	0.144778256239930e+1

Table 1: Parameter sets (Y1-Y3) of the 6th order integrators by Yoshida [8]. w_0 is given by $w_0 = 1 - w_1 - w_2 - w_3$.

3 Efficiency of the HMC algorithm

In order to compare among various integrators one needs a criterion which ranks integrators. Following Ref.[4] we utilize the efficiency function E_{ff} constructed from a product of acceptance P_{acc} and step-size Δt:

$$E_{ff} = P_{acc}\Delta t. \tag{11}$$

This function has one maximum at a certain step-size which we denote Δt_{opt}. Using the energy difference ΔH the acceptance is expressed by [5]

$$\langle P_{acc}\rangle = \mathrm{erfc}(\frac{1}{2}\langle\Delta H\rangle^{1/2}), \tag{12}$$

where erfc is the complementary error function. In stead of using eq.(12), when $\langle \Delta H \rangle$ is small, we may use

$$\langle P_{acc} \rangle = \exp(-\frac{2}{\sqrt{\pi}} \langle \frac{1}{8} \Delta H^2 \rangle^{1/2}). \tag{13}$$

Although mathematically speaking eq.(13) is valid only for $\langle \Delta H \rangle \ll 1$, the numerical study [4] shows that eq.(13) approximates the acceptance quit well for $\langle \Delta H \rangle \leq 3$ which corresponds to $\langle P_{acc} \rangle \geq 20\%$. This is enough for our purpose since typically the acceptance of the HMC is taken to be $\langle P_{acc} \rangle \geq 50\%$.

In the lowest order of Δt, $\langle \Delta H \rangle$ of the n-th order integrator is expressed as [4, 5]

$$\langle \Delta H^2 \rangle^{1/2} = C_n V^{1/2} \Delta t^n + \mathcal{O}(\Delta t^{n+1}), \tag{14}$$

where V is volume of the system and C_n is a Hamiltonian dependent coefficient.

Substituting eq.(14) into eq.(13) one obtains

$$\langle P_{acc} \rangle = \exp(-\widetilde{C}_n V^{\frac{1}{2}} \Delta t^n), \tag{15}$$

where $\widetilde{C}_n \equiv C_n / \sqrt{2\pi}$. If one uses eq.(15) for eq.(11) one can easily obtain the optimal step size which gives the maximum efficiency:

$$\Delta t_{opt} = \sqrt[n]{\frac{1}{n \widetilde{C}_n V^{\frac{1}{2}}}}. \tag{16}$$

Furthermore substituting Δt_{opt} to eq.(15) one obtains the optimal acceptance[2] as

$$\langle P_{acc} \rangle_{opt} = \exp(-\frac{1}{n}) \tag{17}$$

$$= \begin{cases} 0.61 & \text{2nd} \\ 0.78 & \text{4th} \\ 0.85 & \text{6th.} \end{cases} \tag{18}$$

Note that the above result does not depend on the Hamiltonian and can be applied for any model.

Using eq.(16) and (17) we obtains the optimal efficiency of the n-th order integrator:

$$(E_{ff})_{opt}^{n-th} = \exp(-\frac{1}{n}) \sqrt[n]{\frac{1}{n \widetilde{C}_n V^{\frac{1}{2}}}}, \tag{19}$$

We use eq.(19) to compare among integrators. Eq.(19) is easy to handle because eq.(19) has one unknown parameter $\widetilde{C}_n$ and the value of $\widetilde{C}_n$ can be estimated easily from a single simulation on a rather small lattice.

[2] A recent study [11] shows that if one considers higher order effects of Δt the optimal acceptance might be slightly changed. In the current study we omit this small effect.

Now let us compare n-th and m-th order integrators ($n > m$). If one obtains a gain G for the n-th order integrator over the m-th order one, the following condition must be satisfied:

$$(E_{ff})_{opt}^{n-th} = G k_{nm} (E_{ff})_{opt}^{m-th}, \tag{20}$$

where k_{nm} is a relative cost factor needed to implement the n-th order integrator against the m-th one and G is defined so that both n-th and m-th order integrators are equally effective with $G = 1$. In our case, $k_{42} = 3$ and $k_{64} = 7/3$. Substituting eq.(19) to eq.(20) and rewriting the equation one obtains the lattice volume needed to have the gain G:

$$V^{\frac{n}{2}-\frac{m}{2}} = (G k_{nm} \exp(-\frac{1}{m} + \frac{1}{n}))^{nm} \left(\frac{1}{m\widetilde{C}_m}\right)^n (n\widetilde{C}_n)^m. \tag{21}$$

4 Simulation results

We use the plaquette gauge action and standard Wilson fermion action with two flavors of degenerate quarks ($n_f = 2$). We first determine the coefficients C_n at zero and finite temperature. This can be done by measuring $\langle \Delta H^2 \rangle^{1/2}$ at a small step-size and substituting the results into eq.(14). The trajectory length is set to 1. We choose $\beta = 5.75$ and make simulations on both 12^4 and $12^3 \times 4$ lattices. The critical kappa κ_c of $n_f = 2$ at this β is around 0.157[3]. We use several κ's in a range of $0.1 \leq \kappa \leq 0.155$. In this range we maintain the confinement phase on the 12^4 lattice and the deconfinement phase on the $12^3 \times 4$ lattice. In this study we refer to the results on the $12^4(12^3 \times 4)$ lattice as those at zero(finite) temperature.

Figs.1-3 show C_n as a function of $m_q a$. Here $m_q a$ is defined by $m_q a = (1/\kappa - 1/\kappa_c)/2$. At large quark masses where the fermionic effects are negligible, values of C_n at zero and finite temperature coincide each other. This may indicate that the contribution to C_n from the gauge sector is almost same at zero and finite temperature. At small quark masses C_n at zero temperature increases more rapidly than those at finite temperature as $m_q a$ decreases. The quark mass dependence of C_n at finite temperature, compared to that at zero temperature, is small for all the integrators studied here. This behavior is consistent with the result of Ref.[5]. Substituting values of C_n at finite temperature into eq.(21) with $G = 1$, we calculate the lattice size L_e (here $V = L_e^3 \times N_t$). This lattice size L_e is the one with which the higher order integrator and the lower order one perform equally. For a lattice size $L > L_e$ the higher order integrator is more effective than the lower one. Fig.4 shows L_e from comparison between the 2nd and 4th order integrators (2nd vs. 4th) and between the 4th and 6th order ones (4th vs. 6th). For the case of 4th vs. 6th, L_e increases as $m_q a$ decreases, which we do not appreciate. On the other hand for the 2nd vs. 4th, L_e remains less than 20 even at small $m_q a$. This result is contrast to that obtained at zero temperature where L_e increases as $m_q a$ decreases [4]. The above result encourages us to use the 4th order integrator at finite temperature.

[3]This value is estimated from Figure 5 in Ref.[12]

	$18^3 \times 4$		$28^3 \times 4$	
$\kappa = 0.1525$	2nd	4th	2nd	4th
Δt	1/24	1/10	1/36	1/12
Acceptance	0.57(2)	0.81(2)	0.60(3)	0.81(3)

Table 2: Step-size and acceptance at $\kappa = 0.1525$.

The results in Fig.4, however, just show the lattice on which the both integrators are equally effective. To use the higher order integrator in simulations one must obtain some gain over the lower order one. In Fig.5, using eq.(21), we show the expected gain (the region between the solid lines) at $\kappa = 0.1525 (m_q a \approx 0.094)$ as a function of lattice size L. To have $G = 2$ gain (which means 2 times faster) a lattice size $L \approx 100$ is required. This huge lattice size is still not accessible in the current large-scale simulations. Probably the maximum lattice size accessible at the moment is $L \leq 50$. Therefore we can not expect a large gain from the 4th order integrator even if it is used now. If we use a lattice with $L \approx 50$, $G \approx 1.5$ can be achieved. Thus at the level of the current large-scale simulations, we expect to obtain $G \leq 1.5$.

We also make simulations at $\kappa = 0.1525$ to confirm that we can actually obtain a gain for the 4th order integrator over the 2nd one. At $\kappa = 0.1525$, L_e is estimated to be 17.5(9). We choose $18^3 \times 4$ and $28^3 \times 4$ lattices. On the $18^3 \times 4$ lattice we expect $G \approx 1$ and on the $28^3 \times 4$ lattice, $G > 1$. The step-size is adjusted so that the acceptance gives a similar value with eq.(18). The gain G is calculated by

$$G = \frac{(P_{acc} \times \Delta t)_{4th}}{3(P_{acc} \times \Delta t)_{2nd}}, \tag{22}$$

where a factor of 3 in the denominator comes from the relative cost factor $k_{42} = 3$. Table 2 shows the simulation results. Using these results, we obtain $G = 1.08(3)$ on the $18^3 \times 4$ lattice and $G = 1.35(8)$ on the $28^3 \times 4$ lattice (see also Fig.5). As expected the gain increases with L. The result on the $28^3 \times 4$ lattice is an example showing that the 4th order integrator is more effective than the 2nd order one.

5 Conclusions

We studied higher integrators for the HMC algorithm at finite temperature. Contrast to the zero temperature case, the 4th order integrator at finite temperature can be more effective than the 2nd order one. This was demonstrated by the simulations at $\beta = 5.75$ on $L^3 \times 4$ lattices. The gain is dependent of the lattice size. It was shown that on the $28^3 \times 4$ lattice at $\beta = 5.75$ and $\kappa = 0.1525$ the 4th order integrator is about 35% faster than the 2nd order one.

When large-scale simulations at finite temperature are planned, it is recommended to check which integrator is effective for the lattice considered. This check can be done

easily. First we measure C_2 and C_4. This first step does not take much computational time since they can be measured on a small lattice. Then substituting values of C_2 and C_4 to eq.(21), we obtain a relation between G and L. If we obtain $G > 1$ on the lattice planned for the simulations, we should consider to use the 4th order integrator.

Acknowledgments

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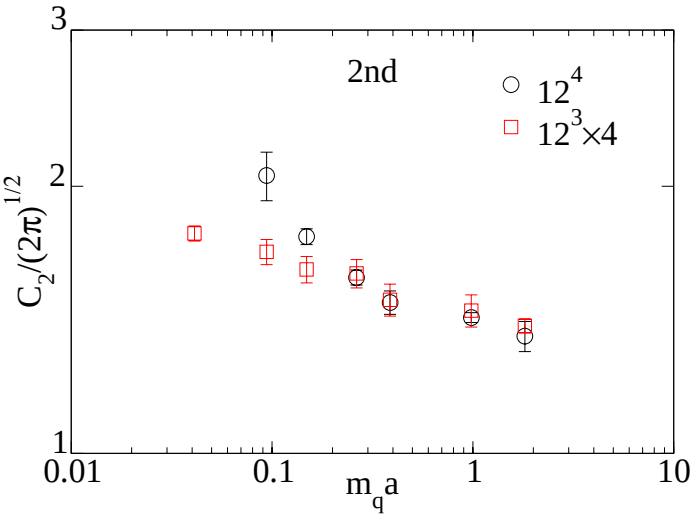

Figure 1: C_2 as a function of the quark mass $m_q a$. In the figure, C_2 is normalized as $C_2/(2\pi)^{1/2} \equiv \tilde{C}_2$.

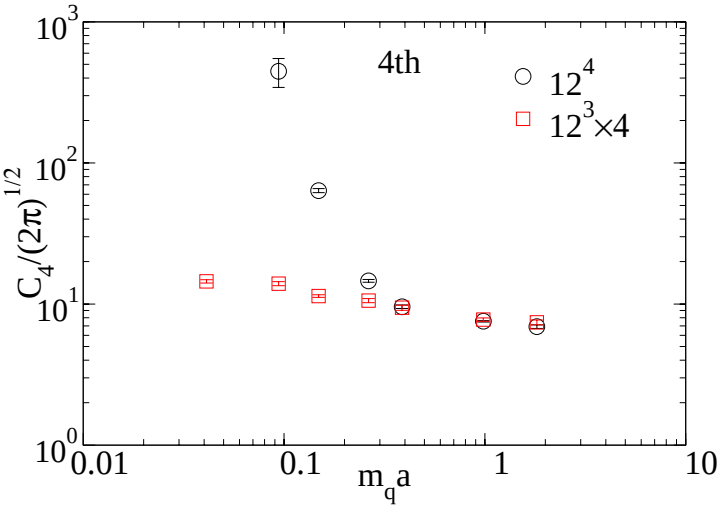

Figure 2: Same as in Fig.1 but for C_4.

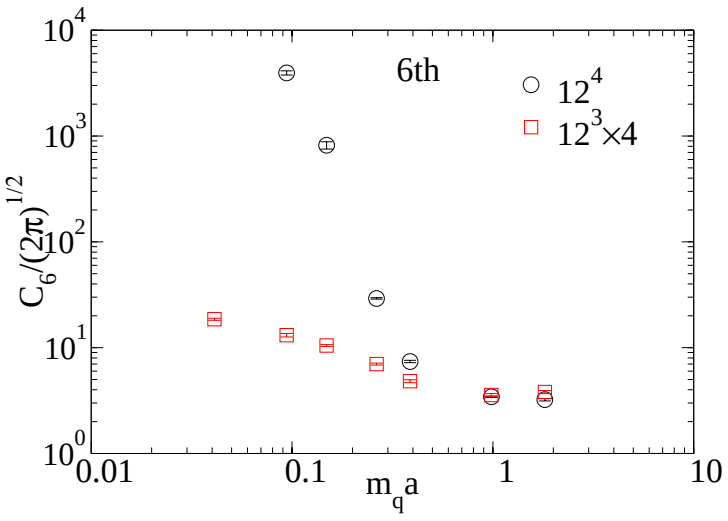

Figure 3: Same as in Fig.1 but for C_6.

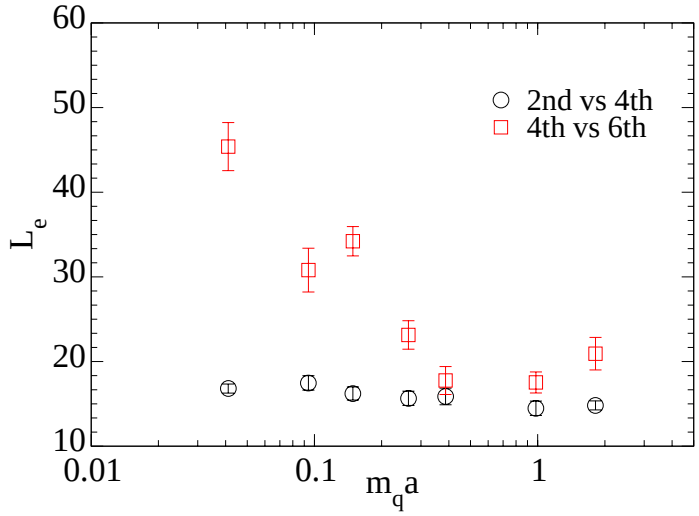

Figure 4: L_e as a function of the quark mass $m_q a$. L_e stands for the lattice size for which the higher order integrator and the lower order one are equally effective. Circles are from comparison between the 2nd order integrator and the 4th order one, and squares are comparison between the 4th order integrator and the 6th order one.

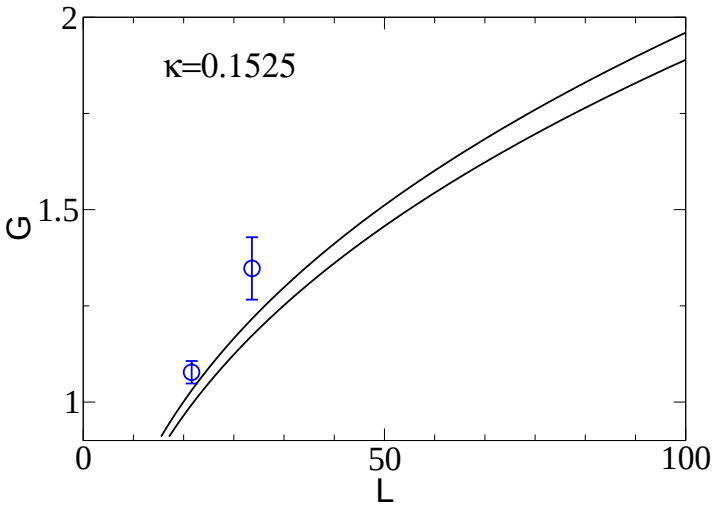

Figure 5: The gain G as a function of L (here $L^3 \times 4$) at $\kappa = 0.1525$. The solid lines are calculated from eq.(21). Circles are from Monte Carlo simulations.